

1,4-Ethanonaphtho(1,8-ef)-1,4-diazepine, 2,3-dihydro-
59950-41-3 | DTXSID40208664

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 329 °C

Global applicability domain: Outside

Local applicability domain index: 3.49e-01

Confidence level: 4.84e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Acibenzolar-S-methyl

Measured: 267

Predicted: 295

[Image not found](#)

1,3-Dimethyl-1,3-diphenylurea

Measured: 350

Predicted: 338

[Image not found](#)

4,4'-Methylenebis(N,N-dimethylaniline)

Measured: 390

Predicted: 349

[Image not found](#)

3,5-Diphenyl-1,2,4-oxadiazole

Measured: 290

Predicted: 317

[Image not found](#)

2-Methyl-5-nitro-1H-isoindole-1,3(2H)-dione

Measured: 361

Predicted: 323